

Thermomechanical Treatment of Fluid-Fluid Interfaces within Density Gradient Theory - A Review

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Density gradient theory (or Cahn-Hilliard theory) has often been used in recent years to calculate density profiles in the three-dimensional microscopic region, which separates fluid phases, and the macroscopic surface tension acting in the interface between the phases. In this theory it is assumed that the local free energy density is composed of two terms, the conventional free energy density as described by the equation of state and an additional term depending on the square of the density gradient. Since the free energy density, here as a function of temperature, density, and density gradient squared, is a fundamental equation of state, all thermodynamic properties can be calculated from it. However, it is not commonly known how this can be done within density gradient theory. In particular, it is not commonly known how the components of the pressure tensor in the interfacial region can be obtained. Moreover, applications have been restricted to interfaces in thermodynamic equilibrium.

By a literature search, it was surprisingly found that a group of French mechanists already had developed a complete 'thermomechanical' density gradient theory in the 1980ies, which provides solutions to these problems. Basis of these works is a fundamental article by Germain [1] on the application of the principle of virtual power in continuum mechanics, which is employed to derive the momentum balance. Based on this work, Seppecher [2] derived the momentum, energy and entropy balances within density gradient theory. As a side product, this derivation yielded the expression for the pressure tensor in the interfacial region. In his postdoctoral thesis [3], Seppecher developed further details of the theory. Jamet [4] and Fouillet [5] applied the theory not only to plane fluid-fluid interfaces, but also to more complex phenomena, such as the formation of a bubble on a hot solid surface. These works will be reviewed and simple illustrative applications will be discussed.

- [1] Germain, *J. Mech.* **12**, 235-274 (1973).
- [2] Seppecher, *These de Docteur de l'Universite Paris VI*, 1987.
- [3] Seppecher, *Universite Paris VI*, 1996.
- [4] Jamet, *These de Doctorat de l'Ecole Centrale Paris*, 1998.
- [5] Fouillet, *These de Doctorat de l'Universite Paris VI*, 2003.